

PROJECT NUMBER: 1752
PROJECT TITLE: Optical Spectroscopy of Tobacco and Smoke
PROJECT LEADER: J. O. Lephardt
PERIOD COVERED: April, 1988

I. TANDEM MASS SPECTROMETRY

- A. Objective: To evaluate for acquisition commercially available tandem mass spectrometer systems.
- B. Results: Discussions were held with the commercial vendors and arrangements were made to visit the facilities of three vendors to conduct performance tests on their equipment. Visits to two vendors have been completed, and the third visit is scheduled for next week.
- C. Conclusions: Distinct differences were found in both the ease of use of the two systems examined thus far and the general operation of the two companies involved. These observations supported the assessments obtained from present users of each companies equipment as to the responsiveness and service records of each company.
- D. Plans: Upon completing the third site visit, assessment of the three system's relative merits for PM applications will be made and preparation of a formal recommendation and purchase request initiated.

II. SMOKE ANALYSIS

- A. Objective: Mainstream smoke analysis of Trim cigarettes.
- B. Results: Test cigarettes, coded P2123-42, G8IS, with a Trim II blend and 35% CaCO₃ of small particle size in the paper were compared with the Kentucky reference cigarettes, 1R4F, by fractionation of the mainstream smoke. In the basic fractions, 22 bases, including some pyridines, pyrazines and most of the minor alkaloids, show small but significant differences between the two cigarettes. The intensities of these compounds, except methylpyrazine and 2,6 dimethylpyrazine, favor the reference cigarette. Among the acidic compounds, 18 components are different including many phenolic compounds, aromatic acids and fatty acids. The intensities of the acidic compounds show more parity in these two cigarettes. In the neutral fraction, significant differences were seen for toluene, indole, 3-methylindole and four megastigmatrienone isomers.
- C. Plans: Continue to provide support as required.
- D. References:

Hsu, F. & M. Buckner, "Mainstream Smoke of Project Trim Cigarettes," memo to R. Cox, April 8, 1988.

- A. **Objective:** Determination of MS and SS Acrolein by TDL Spectroscopy
- B. **Results:** The mainstream acrolein deliveries have been determined for 100% single blend component cigarettes which were part of the training set for the North Complex Smoking Panel. On a per puff basis, 100 % RCB delivered the lowest level (6.5 micrograms/puff) while 100 % ET delivered the highest level (16.1 micrograms/puff). FTR reference cigarettes C20 and C50 delivered approximately 9 and 4.5 micrograms/puff respectively.
- C. **Conclusions:** In MS, acrolein deliveries are not dramatically different relative to the type of tobacco smoked.
- D. **Plans:** The effect of casings and glycerine free blends will be evaluated for MS acrolein. The SS inlet system will be set up and SS measurements for the 100 % single blend components cigarettes will be made. Comparisons with the 2,4 DNPH aldehyde procedure will also be made.
- E. **References:**
- PM Notebook #8617, pp. 1, 2, 9.

- A. **Objective:** To compare the organic gas phase of smoke from Project Trim cigarettes to that from 1R4F control cigarettes.
- B. **Results:** No difference was seen in the OGPP from the Trim cigarettes when compared to the 1R4F controls.
- C. **Conclusions:** The experimental conditions and results were described in a memo.
- D. **References:**
- Magin, D. F., "OGPP Analysis of Project TRIM Cigarettes," memo to R. Cox, April 5, 1988.

III. ASHTRAY ODOR

- A. **Objective:** Fractionation of neutral fraction from ashtray odor.
- B. **Results:** An absorption column packed with 40 um silica gel was used to further fractionate the neutral compounds isolated from cigarette butts. By eluting successively with hexane, methylene chloride, methylene chloride/methanol (9:1 by volume), and methanol, four fractions were obtained. By comparing the GC profiles and the resulting odor from each fraction, the fractionation was fairly reproducible. Fractions 1, 3 and 4 had strong and distinct odors. All four fractions are being evaluated by the Odor Profiling Panel. The compounds in fractions 3 and 4 are being identified by GC/MS analysis.

- C. Plans: The odor intensity of those compounds in fractions 3 and 4 will be evaluated by GC/sniffing/MS. Their retention indices will also be measured and entered into a RS/1 table.

IV. PYROLYSIS-GC/MS

- A. Objective: To examine CR- Compounds using the technique of Curie Point Pyrolysis-GC/MS.

B. Results:

Samples run during the month of April included: CR-2704, -2706, -2722, -2513, -2514 (for J. Paine); CR-2719 (for R. Izac); CR-2643 (for K. Podraza). Each of these was pyrolyzed at two temperatures, the pyrolyzates chromatographed using fused silica capillary column GC, and the peaks detected and identified using mass spectrometry.

In addition, the results of last month's pyrolysis-GC/MS of samples CR-2707, -2708, -2711, and -2712 (for R. Izac), were reexamined in order to determine the ratio of menthol to menthenes and the relative release of menthol upon pyrolysis of these compounds.

- C. Conclusions: The results of these experiments were conveyed to the originators of the samples in memos. The reexamination of the results of the samples from last month was communicated to R. Izac.

D. References:

1. Magin, D. F., "Pyrolysis-GC/MS of CR-2719," memo to R. Izac, April 8, 1988.
2. Magin, D. F., "Pyrolysis-GC/MS of CR- Compounds," memo to J. Paine, April 11, 1988.
3. Magin, D. F., "Pyrolysis-GC/MS of CR-2643," memo to K. Podraza, April 20, 1988.